

## Investigation of the Structure of Barium Modified Zeolite Catalysts

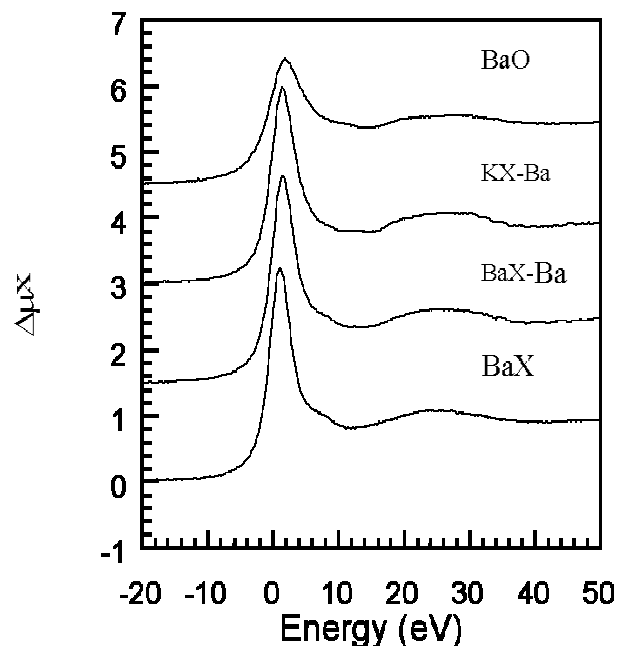
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Beamline(s): X10C

**Introduction:** Ruthenium supported by barium promoted zeolite X is known to be a good catalyst for ammonia synthesis. The traditional iron based catalyst requires high temperatures and pressures to achieve acceptable reaction rates and meet industrial needs. These new ruthenium catalysts have the potential to lower operating costs significantly. Despite their potential, very little is known about these catalysts. We have been using x-ray absorption spectroscopy (EXAFS and XANES) to determine the atomic structure near barium promoters in zeolite X in hopes of elucidating the role of barium in the catalyst.

**Results:** X-ray absorption studies were performed at the Ba  $L_{III}$  edge on barium modified zeolite X in three different ways. Namely, barium solely occluded in the pores of the zeolite framework, barium solely ion exchanged and barium in both ion exchange and occluded sites (as in the active catalyst). Several standard compounds were also analyzed ( $BaO$ ,  $BaCO_3$ ,  $BaSO_4$ ,  $Ba(NO_3)_2$  and  $Ba(OH)_2 \cdot 8H_2O$ ). The XANES spectra, as seen in **Figure 1**, for the three zeolite samples are different from the barium oxide reference after heating to 773K in He and cooling to 298K. Analysis of the threshold energy revealed, as expected, an oxidation state of Ba+2 for each of the catalysts and standards. In general, the white line intensity was found to be greater on the zeolite samples compared to the bulk reference compounds. Results from EXAFS analysis are forthcoming.



**Figure 1.** Ba  $L_{III}$  edge of Ba modified zeolite X supports and BaO standard.